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Gradient Flow Techniques for Multicomponent Diffusion(-Reaction)

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Multicomponent exclusion

Consider process for M+1 different types of particles on lattice (or symmetric graph) with following rule :

If *i* and *j* are on neighbouring lattice sites, they can can change with rate K_{ij}

We think of $i=0$ as the void sites, hence $K_{i0}=K_{0i} > 0$ for all $i =1,..,M$

Multicomponent exclusion

Master equation after mean-field closure

Described by probability to have particle of type *i* at *x*: $u_i(x)$

Master equation

$$\partial_t u_i(x) = \sum_{y \in \mathcal{N}(x)} \sum_j K_{ij}(u_i(y)u_j(x) - u_i(x)u_j(y))$$

Note

$$\sum_i u_i(x) = 1 \qquad \sum_i \partial_t u_i(x) = 0$$

Continuum Limit

Formal limit for shrinking lattice size, local neighbourhoods

$$\partial_t u_i = \sum_j D_{ij} \nabla \cdot (u_j \nabla u_i - u_i \nabla u_j)$$

Rigorous limit for shrinking lattice size, nonlocal neighbourhoods

$$\partial_t u_i(x) = \sum_j D'_{ij} \int (u_i(y) u_j(x) - u_i(x) u_j(y)) \, dy$$

$$= \sum_j D'_{ij} \int (u_j(x)(u_i(y) - u_i(x)) - u_i(x)(u_j(y) - u_j(x))) \, dy$$

Simple exclusion

For M=1 we recover the simple exclusion process

$$\partial_t u_1(x) = \sum_{y \in \mathcal{N}(x)} K_{01}(u_1(y)(1 - u_1(x)) - u_1(x)(1 - u_1(y)))$$

Local continuum limit

$$\partial_t u_1(x) = D_{01} \nabla \cdot ((1 - u_1)\nabla u_1 - u_1 \nabla (1 - u_1)) = D_{01} \Delta u_1$$

Nonlocal continuum limit

$$\partial_t u_1(x) = D'_{01} \int (u_1(y)(1 - u_1(x)) - u_1(x)(1 - u_1(y)))\, dy$$

Gradient Structure, Continuum

Local continuum model

$$\partial_t u_i = \sum_j D_{ij} \nabla \cdot (u_j \nabla u_i - u_i \nabla u_j)$$

Rewritten

$$\partial_t u_i = \sum_j D_{ij} \nabla \cdot (u_i u_j \nabla (\log u_i - \log u_j))$$

Gradient flow

$$\partial_t u_i = \sum_j D_{ij} \nabla \cdot (u_i u_j \nabla (\partial_{u_i} E - \partial_{u_j} E))$$

For entropy

$$E(u) = \sum_i \int u_i \log u_i \; dx$$

Equal Interaction

Special case

$$D_{ij} = D_{ji} = D_i \quad \forall j$$

then

$$\partial_t u_i = D_i \sum_j \nabla \cdot (u_j \nabla u_i - u_i \nabla u_j) = D_i \Delta u_i$$

Perturbation theory for $|D_{ij} - D| < \epsilon$

[Berendsen-mb-Ehrlacher-Pietschmann 18]

$$\partial_t u_i - D\Delta u_i = \sum_j (D_{ij} - D) \nabla \cdot (u_j \nabla u_i - u_i \nabla u_j)$$

Almost equal Interaction

Existence of strong solution for ε sufficiently small

$$\partial_t u_i - D\Delta u_i = \sum_j (D_{ij} - D)\nabla \cdot (u_j \nabla u_i - u_i \nabla u_j)$$

$$u_i \in L^2(0, H^2) \cap H^1(0, T; L^2)$$

Weak strong uniqueness in 1D

[Berendsen-mb-Ehrlacher-Pietschmann 18]

Gradient Structure, Continuum

Entropy dissipation

$$\frac{dE}{dt} = -\sum_{i,j} \int D_{ij} u_i u_j |\nabla(\log u_i - \log u_j)|^2 \, dx$$

$$= -\sum_{i,j} \int D_{ij} \left(\frac{u_j}{u_i} |\nabla u_i|^2 + \frac{u_i}{u_j} |\nabla u_j|^2 - 2\nabla u_i \cdot \nabla u_j \right) \, dx$$

Difficult to obtain general estimates if some cross-diffusion coefficients can vanish

Full interaction

Type *i* interacting with all others

$$D_{ij} \geq D, \quad \forall j$$

Entropy dissipation estimate

$$\sum_j \int D_{ij} u_i u_j |\nabla(\log u_i - \log u_j)|^2 \, dx \geq$$

$$D \sum_j \int \left(\frac{u_j}{u_i} |\nabla u_i|^2 + \frac{u_i}{u_j} |\nabla u_j|^2 - 2\nabla u_i \cdot \nabla u_j \right) \, dx =$$

$$D \int \left(|\nabla \sqrt{u_i}|^2 + \sum_j u_i |\nabla \sqrt{u_j}|^2 \right) \, dx$$

Full interaction

Regularity

$$\nabla u_i, \nabla\sqrt{u_i} \in L^2(0,T;L^2)$$

$$\sqrt{u_i}\nabla\sqrt{u_j} \in L^2(0,T;L^2)$$

$$0 \leq u_i \leq 1$$

$$\partial_t u_i \in L^2(0,T;H^{-1})$$

Aubin-Lions type argument: Compactness

$$u_i \in L^2(0,L^2)$$

$$\nabla(\sqrt{u_i}\sqrt{u_j}) \in L^p(0,T;L^p)$$

Void interaction

Theorem [mb-DiFrancesco-Pietschmann-Schlake 2010]

Let $D_{ij} = 0 \qquad i \neq j, i, j > 0$

Then there exists a global weak solution, which gives entropy dissipation and converges to constant for large time.

Proof:

- Approximation of equation in dual (entropy) variables
- Boundedness by entropy principle
- Above compactness arguments to pass to limit

Direct generalization:

$$D_{ij} = 0 \qquad i \neq j, i, j > m$$

$$D_{ij} > 0 \qquad i \neq j, i \leq m$$

Uniqueness: only for $D_{i0} = D \quad i = 1, \ldots, M$ [Zamponi-Jüngel 2015]

Complete interaction

Theorem [mb-Hopf 2021, in prep]

Let $D_{ij} > 0 \quad \forall i \neq j$

Then there exists a global weak solution, which gives entropy dissipation and converges to constant for large time.

Theorem [mb-Hopf 2021, in prep]

Let $D_{ij} > 0 \quad \forall i \neq j$

If there exists a strictly positive (strong) solution, then there is no other weak solution.

Proof: Based on dissipation of relative entropy between strong and weak solution, following [Hopf 2020]

Open case

So far no global existence in cases where variables cannot be grouped into void-type and solid-type

(Local-in-time existence of classical solutions by Amann‘s theory)

First example for M=4

$$\mathbf{D} = \begin{pmatrix} * & * & * & * & * \\ * & * & * & 0 & * \\ * & * & * & 0 & 0 \\ * & 0 & 0 & * & 0 \\ * & * & 0 & 0 & * \end{pmatrix}$$

Extensions

Straight-forward extension: external potential and mean-field interaction

$$E(u) = \sum_i \int (u_i \log u_i + V_i u_i) \; dx + \sum_i \sum_{j<i} \int (W_{ij} * u_i) u_j \; dx$$

Existence results analogous

Stationary state may change

With confinement convergence to nontrivial states on unbounded domain as well

Pattern Formation, M=1

Gradient flow

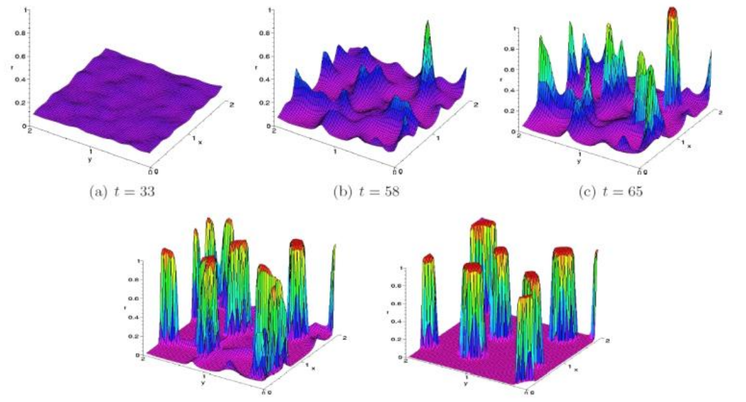
$$\partial_t u_1 = \nabla \cdot (u_1(1 - u_1)\nabla F'(u_1))$$

for entropy-energy

$$F(u_1) = \int u_1 \log u_1 + (1 - u_1)\log(1 - u_1) + \frac{1}{2}\int (W * u_1)u_1 \; dx$$

Attrative interation kernel W

Cluster formation and coarsening in the large time limit



(a) $t = 33$ (b) $t = 58$ (c) $t = 65$

(d) $t = 84$ (e) $t = 250$

Figure 1: Numerical solution of the parabolic system (1)–(4) with random initial data $\varrho_I \in [0.1, 0.11]$ and $\varepsilon = 10^{-4}$.

Multispecies Model

Two-species model $r = u_1, b = u_2, \rho = 1 - u_0$ $K = -W$

$$\partial_t r = \nabla \cdot (\varepsilon(1-\rho)\nabla r + \varepsilon r \nabla \rho + r(1-\rho)\left[\nabla(c_{11} K * r - K * b) + \nabla V\right]),$$
$$\partial_t b = \nabla \cdot (D\varepsilon(1-\rho)\nabla b + D\varepsilon b \nabla \rho + Db(1-\rho)\left[\nabla(c_{22} K * b - K * r) + \nabla V\right])$$

Global existence of bounded weak solutions by gradient flow techniques and boundedness by entropy

[Berendsen-mb-Pietschmann 2017]

Two-Species Cahn-Hilliard

Defining a nonlocal Laplacian (similar *Slepcev 08*)

$$-\Delta_K u = u - \frac{1}{k} K * u. \qquad k = \int_{\mathbb{R}^N} K(x)\, dx$$

the system can be written as

$$\partial_t r = \nabla \cdot (kr(1-\rho)\nabla(c_{11}\Delta_K r - \Delta_K b + \partial_r W(r,b)))$$
$$\partial_t b = \nabla \cdot (Dkb(1-\rho)\nabla(c_{22}\Delta_K b - \Delta_K r + \partial_b W(r,b)))$$

with multi-well potential

$$W(r,b) = \varepsilon(r\log r + b\log b + (1-\rho)\log(1-\rho)) + \frac{c_{11}}{2}r^2 - rb + \frac{c_{22}}{2}b^2 - \frac{c_{11}}{2}r - \frac{c_{22}}{2}b.$$

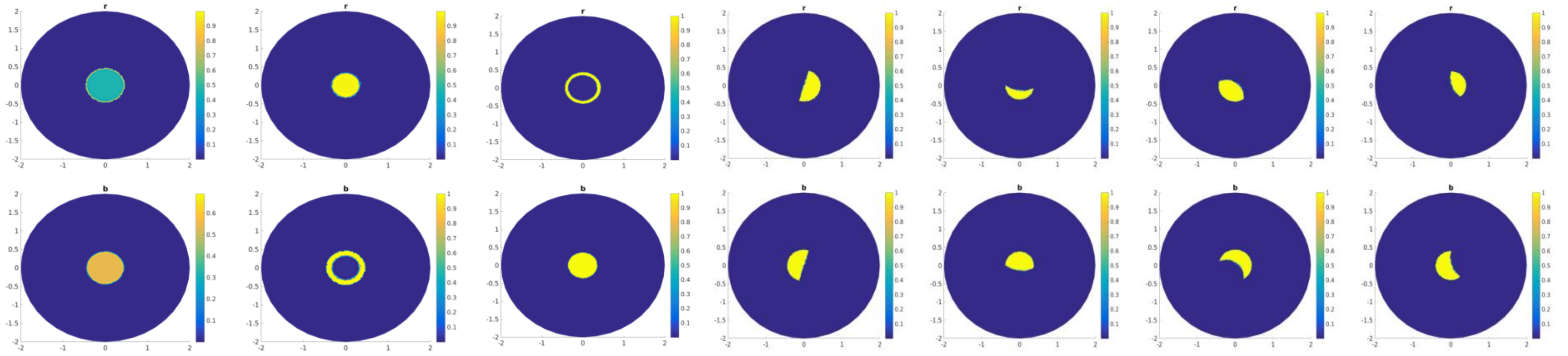
Two-Species Cahn-Hilliard

Convergence to minimizer of the energy minimizer in the large time limit

Gamma-convergence of energy to binary model in the deep-quench limit

Multispecies (nonlocal) isoperimetric problem

Berendsen-mb-Pietschmann 2017, Berendsen-Pagliari 2018



(a) $(c_{11}, c_{22}) = (-0.4, -0.5)$ (b) $(c_{11}, c_{22}) = (-1, -0.5)$ (c) $(c_{11}, c_{22}) = (-1, -3)$ $m_r = 0.2,\ m_b = 0.4$

(a) $(c_{11}, c_{22}) = (-2, -2)$ $m_r = 0.3,\ m_b = 0.3$ (b) $(c_{11}, c_{22}) = (-2, -2)$ $m_r = 0.15,\ m_b = 0.3$ (c) $(c_{11}, c_{22}) = (-2, -1.5)$ $m_r = 0.3,\ m_b = 0.3$ (d) $(c_{11}, c_{22}) = (-2, -1.5)$ $m_r = 0.2,\ m_b = 0.3$

Energy minimizers

Gamma Limit of energy

$$E[\rho] = \int \epsilon(\rho \log \rho + (1-\rho)\log(1-\rho)) + \frac{c_{11}}{2} rK * r + \frac{c_{22}}{2} bK * b - rK * b) \; dx$$

given by

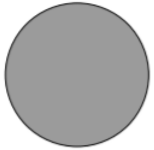
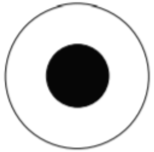
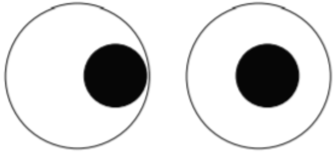
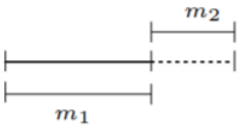
$$E_0[\rho] = \int \frac{c_{11}}{2} rK * r + \frac{c_{22}}{2} bK * b - rK * b) \; dx + \chi(r,b)$$

With characteristic function of admissible set

$$0 \leq r, 0 \leq b, r + b \leq 1$$

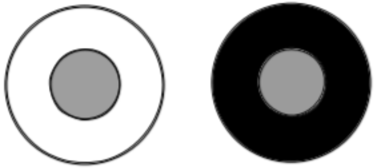
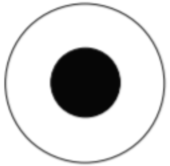
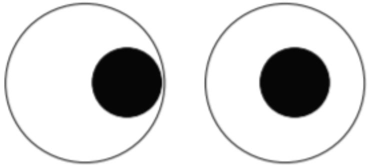
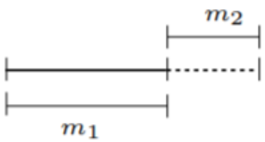
[Cicalese-DeLuca-Novaga-Ponsiglione 2016, Berendsen-mb-Pietschmann 2017]

Radially decreasing K

general K	$-1 < c_{22} \leq 0$	$c_{22} = -1$	$c_{22} < -1$
$-1 < c_{11} \leq 0$	 if $(c_{11}+1)m_1 = (c_{22}+1)m_2$ and K positive definite	?	 if $c_{11}+c_{22} \leq -2$
$c_{11} = -1$	?		
$c_{11} < -1$	 if $c_{11}+c_{22} \leq -2$		 if $N = 1$

Cicalese-DeLuca-Novaga-Ponsiglione 2016

Radially decreasing K

K Coulomb	$-1 < c_{22} \leq 0$	$c_{22} = -1$	$c_{22} < -1$
$-1 < c_{11} \leq 0$			
$c_{11} = -1$			
$c_{11} < -1$			 if $N = 1$

Cicalese-DeLuca-Novaga-Ponsiglione 2016

Microscopic model

Gradient structure of the microscopic model (and similar nonlocal model)

$$\partial_t u_i(x) = \sum_{y\in\mathcal{N}(x)} \sum_j K_{ij}(u_i(y)u_j(x) - u_i(x)u_j(y))$$

Reminder: gradient structures for linear Markov chains

[Zimmer et al 2017, Maas-Mielke 2020, Peletier et al 2020]

$$\partial_t u(x) = \sum_{y\in\mathcal{N}(x)} (u(y) - u(x))$$

$$\begin{aligned}\partial_t u(x) &= \sum_{y\in\mathcal{N}(x)} \sqrt{u(x)u(y)}\,\sinh(\frac{1}{2}(\log u(y) - \log u(x)) \\ &= -\frac{1}{2}D^*(M(u)\sinh(\frac{1}{2}D(\log u)))\end{aligned}$$

Microscopic model

Gradient structure of the microscopic model (and similar nonlocal model)

$$\partial_t u_i(x) = \sum_{y \in \mathcal{N}(x)} \sum_j K_{ij} \sqrt{u_i(x)u_i(y)u_j(x)u_j(y)} \sinh(\frac{1}{2}(\log u_i(y) - \log u_i(x) - \log u_j(y) + \log u_j(x)))$$

$$\partial_t u_i(x) = -\sum_j D^*(M_{ij}(u) \sinh(\frac{1}{2}(D \log u_i - D \log u_j(y))))$$

$$M_{ij}(u) = \frac{K_{ij}}{2} \sqrt{u_i(x)u_i(y)u_j(x)u_j(y)}$$

$$\frac{dE}{dt} = -\sum_j \sum_x M_{ij}(u)(D \log u_i - D \log u_j) \sinh(\frac{1}{2}(D \log u_i - D \log u_j))$$